Combination of Simulations and Data Science to Determine Appropriate Thermocouple Positions in a Crystal Growth Furnace

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In order to produce high quality silicon ingots for solar cells, fine control of growth conditions such as temperature distribution and crucible position is necessary. For this issue, it is important to measure the temperatures along the crucible using thermocouples (TCs) in the appropriate positions and to predict the temperature distribution inside the crucible. In this research, to determine the appropriate TC positions, a combination of crystal growth simulation and machine learning with neural network (NN) was studied.

The crystal growth simulation was conducted using CGsim software modeling our existing furnace, which is based on a silica crucible of 200*135*135 (mm) and 3 heaters in vertical configuration (**Fig.1a**). Simple conditions, steady state and the crucible contains only solid silicon, were used to increase the number of simulation. The total number of calculations was 195, in which the simulations had variations in crucible position and in temperature in the heaters H1 (top) and H2 (middle), and the temperature was fixed for the bottom heater.

Using the simulation data, we made a NN model to predict continuous temperature distribution along the crucible wall from selected 3 temperatures, which correspond to the measured temperatures at TC positions. The NN consisted of 7 inputs (Heater temperatures: H1, H2 and H3, TC temperatures: TC1, TC2 and TC3, and Crucible position), 2 hidden layers with 32 nodes, and 21 outputs (temperature distribution, from 0 to 200 mm with 10 mm step above the crucible bottom). The NN was learned with a batch size of 1000 and for 10000 epochs. Totally, 1329 NNs were tested for the combinations of 3 TC positions from 21 positions along the crucible wall. The appropriate TC positions at 0, 10 and 180 mm were obtained as the minimum loss. These positions are related to discontinuous thermal conductivity at the different materials.

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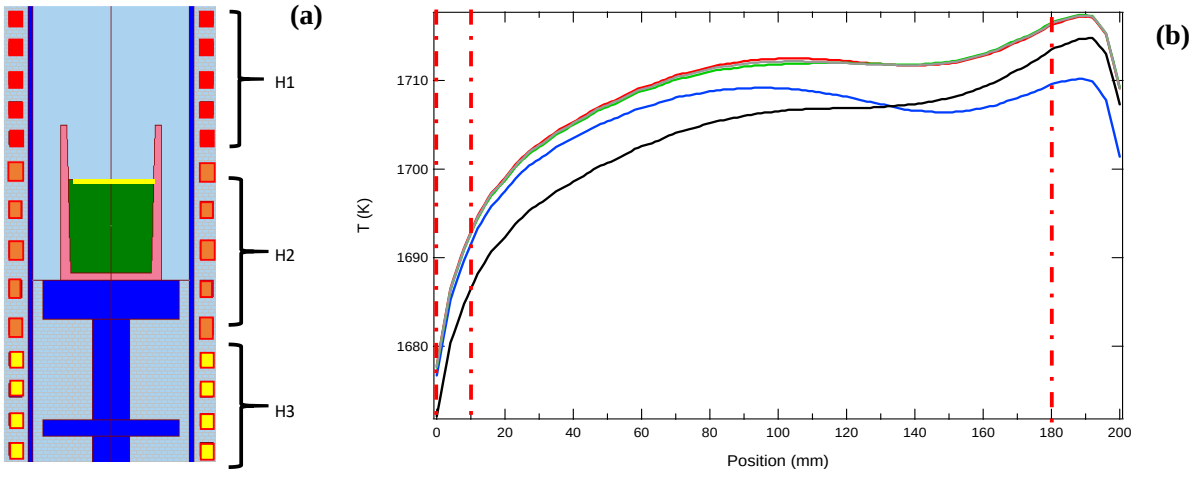

Fig. 1. (a) Schematic illustration of inside the furnace. (b) Examples of temperature distribution along the crucible wall. Dot-and-dash lines indicate appropriate TC positions.